DY 61: Poster - Glasses

Time: Thursday 16:00–18:00 Location: Poster A

DY 61.1 Thu 16:00 Poster A

Molecular dynamics simulation of Two-Dimensional silica using multi-body potentials. — •Projesh Kumar Roy[1] and Andreas Heuer[2] — [1]Institute of Physical Chemistry, University of Muenster. — [2]Institute of Physical Chemistry, University of Muenster.

The discovery of a new material called "Two-dimensional silica bilayer"[1][2]; has created a great excitement among the glass scientists. Using STM and SPM method it was revealed that the material consists of only two atomic layers of silica. It behaves like a 2-D system due to a very remarkable symmetry present between the layers. Under different reaction condition both crystalline and amorphous form was produced separately and sometimes both in the same layer. The nature of the amorphous form is very similar to the Zacharisen's 2D silica glass model. Earlier a "Soft-Core Yukawa"[3] type potential was used to a 2-D model of silica bilayer to describe this structure formation in amorphous state by energy minimization method of the "Inherent Structures"[4]. For a stable 3D model; a continuous surface potential, a gravitational field, and a multi-body potential; such as Stillinger-Weber type three body potential [5]; was used. The system was simulated in various temperatures in NVT. Thermodynamic and kinetic properties of the system were studied and a crystal amorphous transition was characterized.[1]Heyde M. et al,Chem.Phys.Lett. 550,1(2012).[2]HuangP.Y. et al,Nano Lett.,12,1081(2012 [3]Mendez-Maldonado et al.,J.Chem.Phys.137,054711(2012).[4]Stillinger F. et al,Phys.Rev.A 25,2,978(1982). [5]Feuston B.P. et al,J.Chem.Phys,89,9(1988).

DY 61.2 Thu 16:00 Poster A

Influence of Atomic Tunneling Systems carrying a Large Nuclear Quadrupole Moment on the Dielectric Properties of Glasses at Very Low Temperatures — •Annina Luck, Nils Hauff, Anne Zeissner, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

Glasses containing significant amounts of isotopes carrying large nuclear electric quadrupole moments show very surprising effects that are not explained by the standard tunneling model. These effects appear in dielectric measurements, both in the low frequency and the microwave regime.

The nucleus of ^{165}Ho carries a very large electric quadrupole and therefore appears to be a good candidate to investigate the influence of atomic tunneling systems carrying a large nuclear quadrupole moment on the dielectric properties of glasses down to very low temperatures. Here, we present measurements of dielectric properties of the multicomponent glass HY-1, containing several percent of holmium. These measurements have been performed in a wide frequency range from 60 Hz to 1 GHz and at temperatures between 7 mK and several Kelvin.

Our measurements show surprising temperature, frequency and electric field strength dependent effects that indicate a non-phonon based thermal relaxation process.

DY 61.3 Thu 16:00 Poster A

Effects of Confinement on the Dynamics of Aqueous Mixtures — •Matthias Sattig and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt

The dynamical behavior of aqueous mixtures in bulk and in confinement is a topic of great interest. For example, a water concentration dependent behavior of the glass transition temperature was found in PG-water and in PGME-water mixtures, which is very different for the two cases [1]. This was attributed to different possibilities of both molecules to form H-bonds in the bulk and different mechanisms of H-bonding in the presence of additional water. The forming of H-bonds can be disturbed by introducing a geometrical confinement, whose surface interacts with the guest molecules and spatially restricts the bond network. We present rotational correlation times τ of both above mentioned mixtures in bulk and in mesoporous silica MCM-41 at several water concentrations, obtained from ^{2}H-NMR. In the high temperature regime spin-lattice-relaxation experiments show similar results for both mixtures in bulk and in confinement. At lower temperatures they hint at the occurrence of a phase separation, assisting the interpretation from Elamin et al. [2]. They propose the idea of water clustering at the surface. Our results are compared with results from dielectric spectroscopy of the mixtures in bulk and confinement. Similarities with water confined in MCM-41 are discussed, where the observable relaxation at low temperatures was attributed to surface layer of water[3].

[1] Sjöström et al., PCCP, 12, 10452, 2010 [2]; Elamin et al., to be published; [3] Sattig et al., PCCP,16, 19229 , 2014

DY 61.4 Thu 16:00 Poster A

Theory of heterogeneous viscoelasticity — •Walter Schirmacher[1,2,3], Giancarlo Ruocco[3], and Valerio Mazzone[3] — [1]Universität Innsbruck — [2]Universität Mainz — [3]Università "La Sapienza" Roma

We present a new theory of viscoelasticity of a glass-forming viscous liquid near and below the glass transition. In our model we assume that each point in the material has a specific viscosity, which varies randomly in space according to a fluctuating activation free energy. We include a Maxwellian elastic term and assume that the corresponding shear modulus fluctuates as well with a similar distribution as that of the activation barriers. The model can be mapped to an effective heterogeneous elasticity theory, which is solved in coherent-potential approximation (CPA). The theory predicts an Arrhenius-type temperature dependence of the viscosity in the vanishing-frequency limit, independent of the distribution of the activation energies. It is shown that this activation energy is generally different from that of a diffusing particle with the same barrier-height distribution. At finite, but low frequencies the theory describes low-temperature alpha relaxation together with the beta wing. Good agreement with data on metallic glasses is obtained. At high frequencies the theory reduces to heterogeneous elasticity theory, which explains the occurrance of the boson peak and related vibrational anomalies.